

The γ -irradiation Effect on the Optical Properties of CdTe Thin Films Deposited by Thermal Evaporation Technique

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CdTe thin films of 50 nm thickness have been deposited on glass substrates by thermal vacuum evaporation technique and the γ -irradiation effect on their optical properties has been investigated. Transmittance and reflectance have been measured at normal incidence, in the visible region from 400 to 700 nm, and were used to evaluate the optical parameters and the band gap energy for CdTe thin films before and after γ -irradiation. Structure and surface morphology before and after γ -irradiation were investigated using X-ray diffraction (XRD) analysis and scanning electron microscope (SEM) respectively. XRD pattern of the as-deposited CdTe film shows an amorphous nature. Crystalline structure was observed to improve when samples were exposed to γ -irradiation at doses from 40–120 kGy in the (111) plane of the cubic zinc-blende structure. SEM shows a change in the surface morphology of CdTe films as a consequence of γ -irradiation compared to as-deposited sample. The optical properties such as refractive index, extinction coefficient, dielectric constant were found to decrease with the increase of the dose of γ -irradiation. Energy band gap was found to decrease from 2.47 eV for the as-deposited down to 2.20 eV for 120 kGy (blue shift compared to bulk CdTe), that was attributed to the small thin film thickness.

Keywords: cadmium telluride, thin films, optical properties, γ -irradiation.

1. INTRODUCTION

Cadmium telluride (CdTe) has received the attention of scholars for several decades due to its attractive electrical and optical properties. Furthermore, CdTe has a low sublimation temperature that makes it a suitable candidate for physical vapor deposition techniques such as thermal evaporation method [1]. Therefore, it became one of the most promising candidates for optoelectronic applications such as photovoltaic cells accompanied with low cost and good efficiency [2–4], nonlinear integrated optical devices [5], light emitting diodes [6], photometers and radiometers devices such as IR detectors, X-ray detectors, gamma-ray detectors [7–9] and electronic applications such as field effect transistors [10].

Optical properties and the structure of CdTe thin films were found to have a direct dependence on the film's thickness as reported by Lalitha et al. [11], and Patil et al. [12]. Kim et al. [13] studied the effect of annealing temperature on the optical properties of the CdTe thin films. Rahman et al. [14] showed that better films structure and optical properties can be achieved by increasing the annealing time. On the other hand, exposing CdTe to gamma radiation leads to a change in its structural and electrical properties as reported by Maity et al. [15].

Previous studies on CdTe thin films were focused on the variation of structure and optical properties with deposition conditions such as deposition time rate [16], substrates temperature [17], the film's thickness [18, 19]. and the

source temperature [20]. In this work, we studied the optical properties and the optical parameters of very thin films of CdTe (50 nm) when exposed to different doses of γ -irradiation. Very thin films are important in solar cell fabrication based on CdTe semiconductor. Understanding the effect of γ -irradiation on the structure and optical properties such as band gap, refractive index, absorption coefficient, and dielectric constant (real and imaginary parts) of CdTe thin film without pre-annealing is important for fabrication of cheap and efficient optoelectronic and electronic applications.

2. EXPERIMENTAL DETAILS

Glass substrates (2 × 2 cm) were cleaned by acetone, methanol, and distilled water respectively. CdTe powder (99.999 % pure, purchased from Balzers), was evaporated using thermal evaporation technique at room temperature and under a pressure of 8×10^{-8} torr. The evaporation rate was set at 5 Å/s and a film's thickness of 500 ± 2 Å was achieved and measured using the quartz crystal monitor (QCM). The films were irradiated with 1.25 MeV γ -rays using the Co⁶⁰ source at Jordan Atomic Energy Commission. The irradiation dose was varied from 40 to 120 kGy.

The transmission and reflection were measured in the visible wavelength range of 400–700 nm at nearly normal incidence using FilmTek 3000 system (SCI) and Cary 50 ultraviolet-visible (UV-vis) double beam spectrophotometer

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(Agilent). The average error in measuring the reflection and transmission was estimated to be $\pm 4\%$.

The optical parameters such as absorption coefficient (α), extinction coefficient (k), and the refractive index (n) were calculated using the following equations [21–24]:

$$\alpha = \frac{1}{t} \ln \left[\frac{(1-R)^2}{2T} + \left[\left(\frac{(1-R)^2}{2T} \right)^2 + R^2 \right]^{\frac{1}{2}} \right]; \quad (1)$$

$$k = \frac{\lambda \alpha}{4\pi}; \quad (2)$$

$$n = \left(\frac{1+R}{1-R} \right) + \left[\left(\frac{4R}{(1-R)^2} \right) - k^2 \right]^{\frac{1}{2}}, \quad (3)$$

where (t) is the sample thickness, (T) and (R) are the transmission and the reflection coefficient respectively. Furthermore, the real and the imaginary parts of the dielectric constant (ϵ' and ϵ'' respectively), were calculated using the following equations [25, 26]:

$$\epsilon' = n^2 - k^2; \quad (4)$$

$$\epsilon'' = 2nk. \quad (5)$$

3. RESULTS AND DISCUSSION

The typical X-ray pattern for CdTe's cubic structure (zinc-blende) was reported to be observed at $2\theta = 23.7^\circ$, 39.3° , and 46.6° , which corresponds to diffraction peaks from (111) and (220) and (311) planes respectively according to JCPDS file no. 15-0770.

The XRD pattern for our samples before (as-deposited) and irradiated by different doses are shown in Fig. 1. An amorphous nature was observed for the as-deposited (non-irradiated) as shown in Fig. 1 a, the broad peak between 20° – 30° which is usually observed in glass's x-ray diffraction pattern [27], that could be related to substrate's scattering because of the small CdTe thickness (50 nm) [28]. The x-ray pattern for the irradiated samples, shows an increase in the crystalline nature due to irradiation; the preferred orientation peak at $2\theta = 23.7^\circ$ confirms the creation of cubic zinc blend structure [29]. It can be observed that the peak's intensity is increasing and becomes sharper as the irradiation dose increases. The increase in the peak's intensity has been approved to be related to the enhancement of crystals growth and the grain size in the irradiated films [29, 30]; other peaks for CdTe such as (220) and (311) planes are weak, the one intense peak is suggesting a disordered nature of the system. Another peak was observed at $2\theta = 28.88^\circ$ which could be related to the substrates -Si glass (111)- according to JCPDS file no. 27-1402 or corresponds to the (102) plane, which usually observed in the annealed CdTe films as reported by [31]. The effect of γ -irradiation on the CdTe thin film's surface shows random deformations as shown in Fig. 2 (b–80 kGy, c–100 kGy and d–120kGy) respectively. The irradiated samples became darker as the dose of irradiation increases compared to the as-deposited thin film as shown in Fig. 2 a. There was no systematic correlation between the absorbed dose and the distribution of the deformation spots observed on the thin film surface. Scanning Electron Microscopy (SEM) was then used to further assessment of the CdTe thin

film's surface morphology before and after irradiation. Fig. 2 a shows a smooth surface morphology with pinholes were observed for as-deposited (without irradiation). Pinholes are usually observed for imperfect coalescence of the CdTe grains during deposition especially for small thin films thicknesses as in our present work. Fig. 2 b shows a rough and spotting surface of irradiated CdTe thin film at 80 kGy, which could be attributed to the interaction of energetic γ -ray photons with atoms in its path. Therefore, excitation and ionization resulted in the material's atoms that cause a change in the materials structure [32, 33].

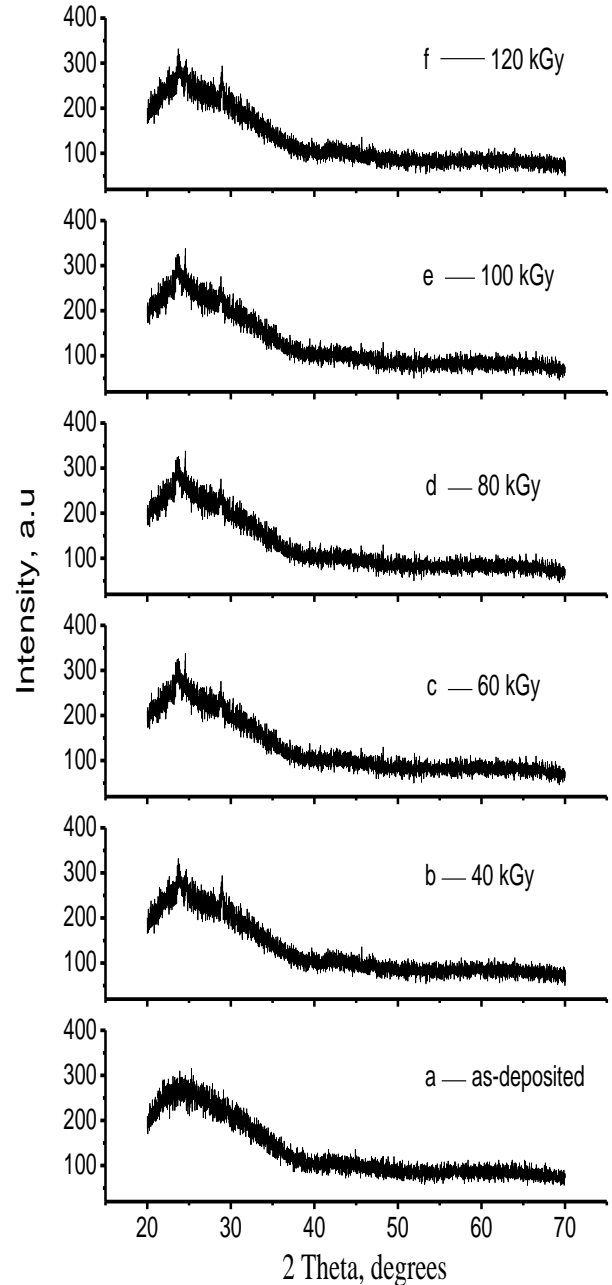


Fig. 1. The XRD patterns for CdTe thin films: a–as-deposited, and γ -irradiated with doses b–40 kGy; c–60 kGy; d–80 kGy, e–100 kGy; f–120 kGy

Fig. 4 a shows that the transmittance of irradiated samples is increasing compared to the as-deposited sample, while the reflectance of the irradiated samples is decreasing as shown in Fig. 4 b.

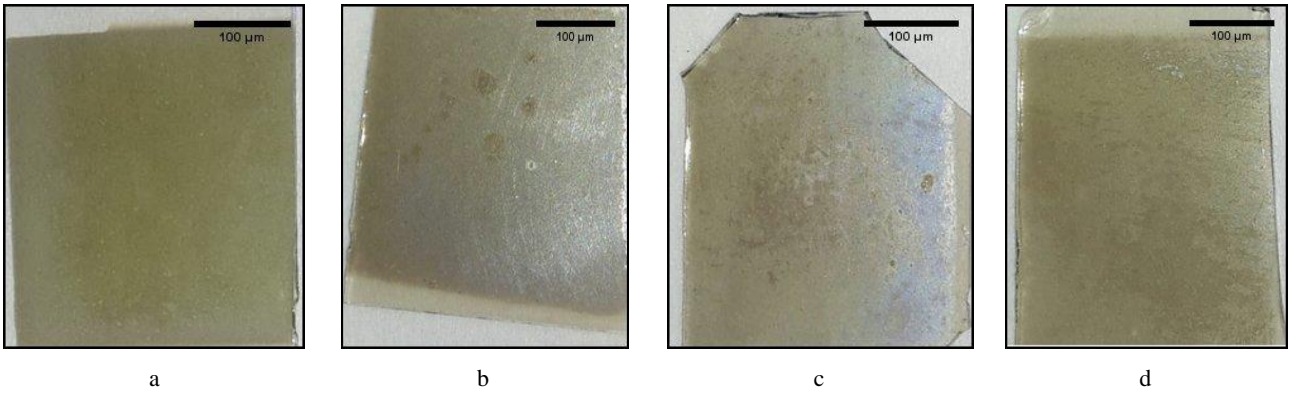


Fig. 2. Camera images show the effect of γ -irradiation on the CdTe thin film's surface: a – before irradiation (as-deposited) and after irradiation at b – 80 kGy; c – 100 kGy; d – 120 kGy

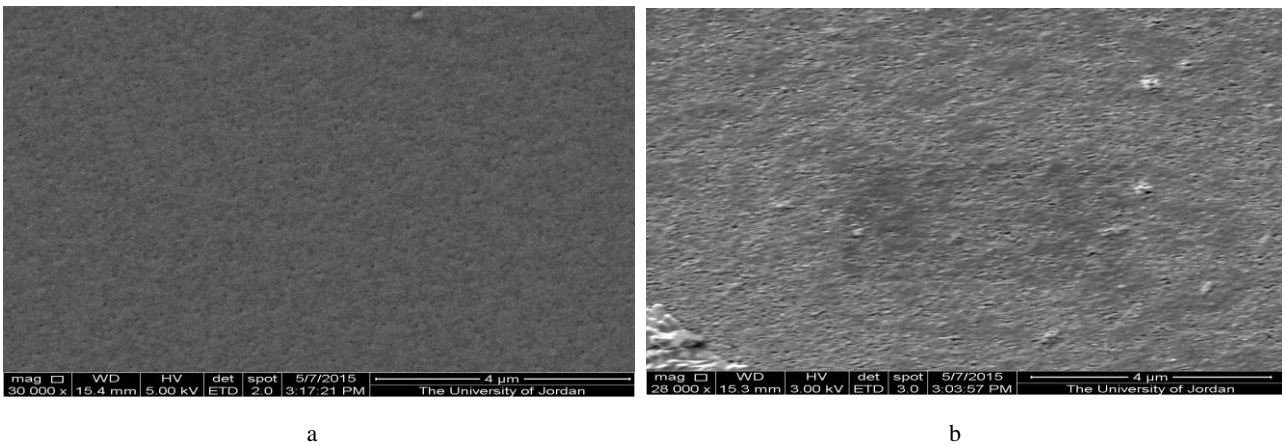


Fig. 3. Scanning electron microscopy (SEM) images show the surface morphology of CdTe films: a – before (as deposited) and b – after γ -irradiation at 80 kGy

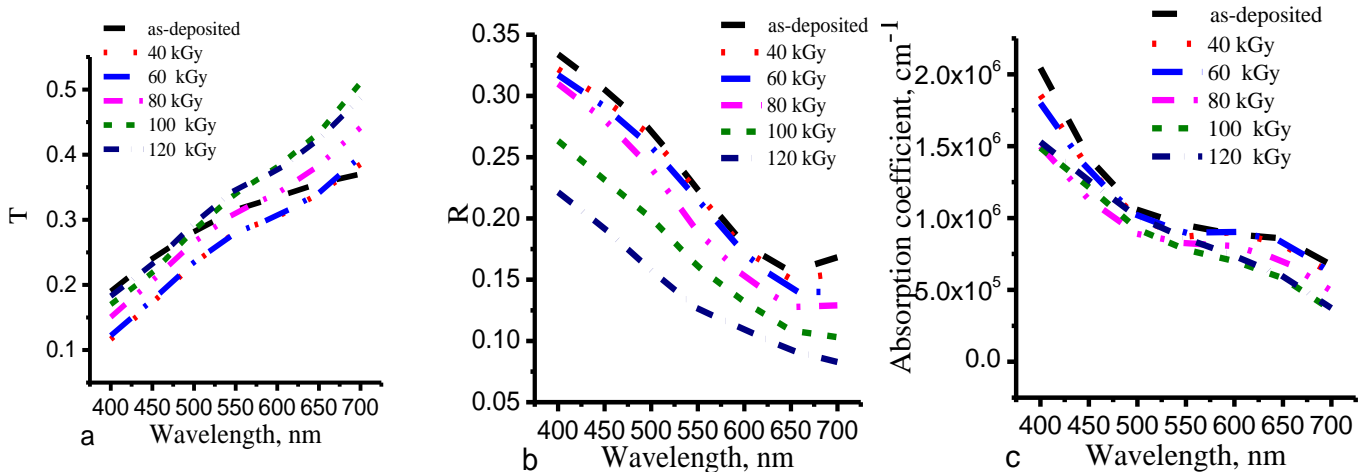


Fig. 4. a – transmission; b – reflection; c – absorption coefficient of CdTe thin films as a function of wavelength

No substantial changes in transmittance and reflectance were observed for the samples irradiated at 40 kGy and 60 kGy, while the effect of irradiation was clearly observed for the samples irradiated at 80–120 kGy. At low wavelength (high photon energy), the absorbance of the irradiated samples has slightly lower values compared to the as-deposited samples, while at high wavelengths (low photon energy) the values are lower. The absorption

coefficient is also decreasing as the wavelengths increases as shown in Fig. 4 c.

The refractive index n values are decreasing as the wavelength increases as shown in Fig. 5 a. It can be observed that refractive index is decreasing as the irradiation dose increasing, which supports that the material became more transparent as the irradiation dose increases, consistent with what have been observed in the

transmittance behavior. The extinction coefficient k was also found to decrease with increasing wavelength and its values were lower than the as-deposited sample as shown in Fig. 5 b. Both parameters n and k don't have a well-defined maximum or minimum as a function of the wavelength, except a little kink at between 600–650 nm, which represents the absorption edge [24]. Refractive index varies in the range from ~ 2 to ~ 4 , while the extinction coefficient varies from ~ 0.1 to ~ 0.65 as a function of wavelength for different doses of irradiation. Table 1 shows the variation of n and k at $\lambda = 550$ nm.

Table 1. The real part of the dielectric constants (ϵ'), the absorption coefficient (α), refractive index (n), and the extinction coefficient (k) at $\lambda = 550$ nm

Dose, kGy	ϵ'	$\alpha \times 10^5, \text{cm}^{-1}$	n	k
0	7.24	9.50	2.721	0.410
40	7.24	8.71	2.716	0.376
60	6.96	8.97	2.666	0.387
80	6.01	8.23	2.477	0.355
100	5.07	7.79	2.276	0.337
120	3.91	8.50	2.012	0.370

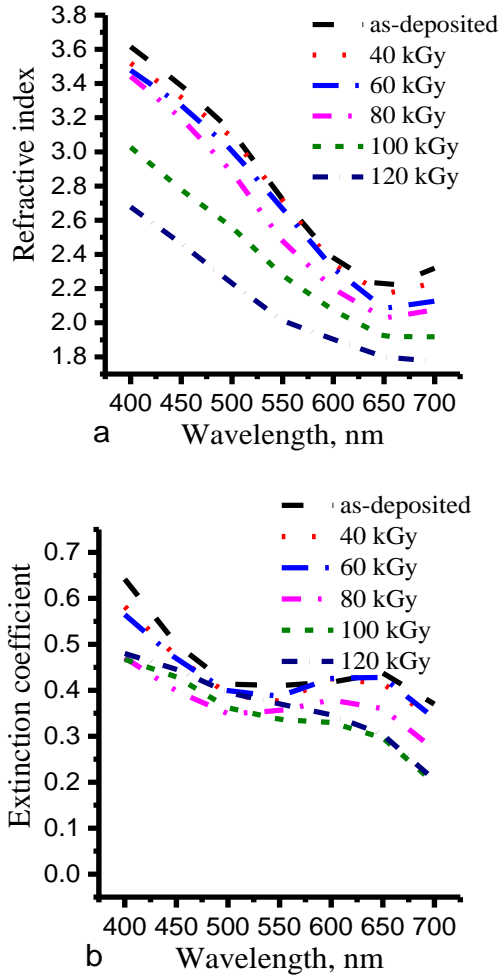


Fig. 5. a–refractive index; b–extinction coefficient versus wavelength for as-deposited and γ -irradiated CdTe thin films

The behavior and values of n and k -at a similar range of the wavelengths- for the as-deposited sample were consistent with what reported by scholars such as Lalitha et

al. [34], El-Shazly and El-Shair [35] and Punitha et al [36]. The variation in k and n values with irradiation reveals that there is a structural change in the films.

Refractive index and extinction coefficient values were used to calculate the real (ϵ') and the imaginary parts (ϵ'') of the dielectric constant. The real part (ϵ') was found to decrease with increasing wavelength and the dose of γ -irradiation as shown in Fig. 6 a. The behavior and values of ϵ' were almost consistent with the calculated values of ϵ' by Kim et al. [13], using the spectroscopic ellipsometry. Table 1 shows the effect of irradiation dose on the real dielectric constant ϵ' at $\lambda = 550$ nm. On the other hand, the imaginary part of the dielectric constant ϵ'' was decreasing with increasing the wavelength and the dose of γ -irradiation as shown in Fig. 6 b.

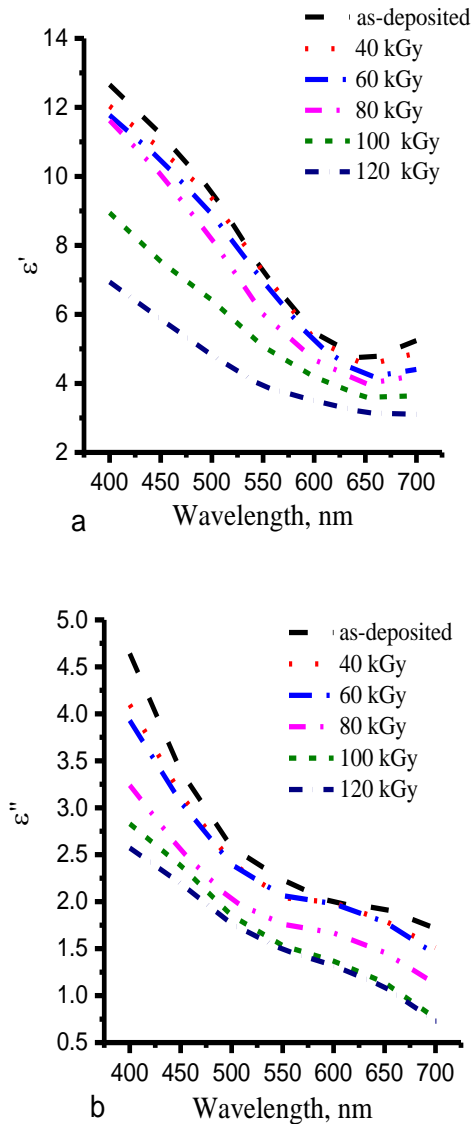


Fig. 6. a–dielectric constants (ϵ'); b–the imaginary part of the dielectric constant (ϵ'') as a function of the wavelength for CdTe thin films

The absorption coefficient is related to the incident photon energy($h\nu$) by [29]:

$$ah\nu = A(h\nu - E_g)^m, \quad (6)$$

where A is a parameter that depends on the transition probability, h is the Planck's constant, ν is the frequency of the light, m is a fitting parameter that takes values 0.5, 1, 1.5, 2 and 3, depending on the type of electron transition and E_g is the energy band gap. We found the best fitting is when $m = 0.5$ which is consistent with the literature [37–39]. Eq. 6 was used to find the optical gap (E_g) by extrapolation the straight line toward the abscissa ($(ah\nu)^2 = 0$), as shown in Fig. 7. The higher value of E_g was recorded for the as-deposited thin film, which recorded a value of 2.47 eV compared to the bulk CdTe band gap which is known as ~ 1.5 eV (a blue shift) [24, 38]. The calculated values of band gap energies were very close to the that values reported for the nano-structure size of CdTe which could be because of the small film thickness. A small grain size and an existence of strain in the structure are expected due to the small thickness of the thin film [40, 41]. The recorded band gap energy values for our studied CdTe thin films make it an appropriate candidate for the fabrication of electroluminescent display devices [41, 42]. Table 2 shows the values of the E_g , where they depend on the irradiation dose; the energy gap decreased from (2.47 eV) for non-irradiated CdTe thin film to (2.20 eV) for the 120 kGy dose of irradiation. The decrease in the band gap energy could be attributed to the increasing of crystallinity as confirmed by the XRD measurements. The irradiation could introduce new energy levels in the forbidden gap which causes radical changes in the carrier concentration in the material [43].

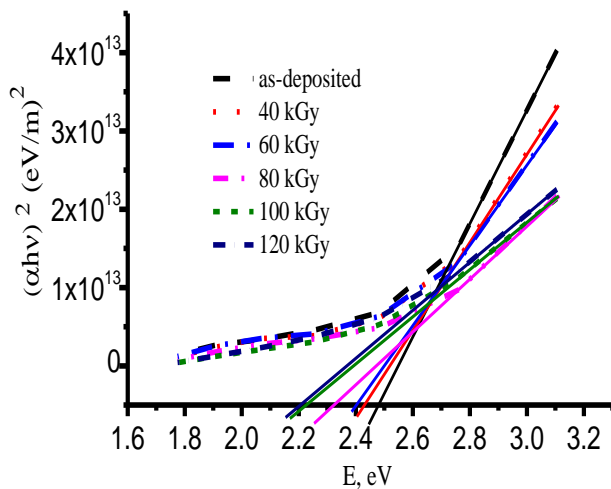


Fig. 7. The band gap energy of as-deposited and γ -irradiated CdTe thin films

Table 2. Band gap energy of CdTe at different irradiations

Dose, kGy	Band gap energy, eV
0	2.47
40	2.43
60	2.40
80	2.31
100	2.22
120	2.20

4. CONCLUSIONS

The effect of γ -irradiation on the CdTe thin films (50 nm) deposited by thermal vacuum evaporation technique on glass substrates were studied. It was found that

exposing CdTe thin films to γ -irradiation helps to improve its structure from an amorphous phase into a crystalline structure in the (111) plane of the cubic zinc-blende structure. The SEM images show a change in the surface morphology as a consequence of γ -irradiation compared to as-deposited sample. Optical parameters were studied in the spectral range from 400 to 700 nm. It was found that transmittance was increasing and reflectance was decreasing with increasing the dose of γ -irradiation. Furthermore, refractive indices, extinction coefficients, absorption coefficient and dielectric constant were decreased, as the dose of irradiation increase, due to the change in the material's structure. Energy band gap (E_g) was found to decrease from 2.47 eV for the as-deposited down to 2.20 eV for 120 kGy (blue shifted compared to bulk CdTe), that could be attributed to the formation of small grain size because of the small thin film's thickness. The small thickness of CdTe and the resulted energy gaps before and after γ -irradiation could be used to fabricate optoelectronic applications with higher energy band gap such as electroluminescent display devices.

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